POLYTOPIC VECTOR ANALYSIS IN IGNEOUS PETROLOGY: APPLICATION TO LUNAR PETROGENESIS.

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Lunar samples represent a heterogeneous assemblage of rocks with complex inter-relationships that are difficult to decipher using standard petrogenetic approaches. These inter-relationships reflect several distinct petrogenetic trends as well as thermo-mechanical mixing of distinct components. Additional complications arise from the unequal quality of chemical analyses and from the fact that many samples (e.g., breccia clasts) are too small to be representative of the system from which they derived.

Polytopic vector analysis (PVA) is a multi-variate procedure used as a tool for exploratory data analysis [1-3]. PVA allows the analyst to classify samples and clarifies relationships among heterogenous samples with complex petrogenetic histories. It differs from orthogonal factor analysis in that it uses non-orthogonal multivariate sample vectors to extract sample endmember compositions. The output from a Q-mode (sample based) factor analysis is the initial step in PVA. The Q-mode analysis, using criteria established by Miesch [4] and Klovan and Miesch [5], is used to determine the number of endmembers in the data system. The second step involves determination of endmembers and mixing proportions with all output expressed in the same geochemical variable as the input. The composition of endmembers is derived by analysis of the variability of the data set. Endmembers need not be present in the data set, nor is it necessary for their composition to be known a priori. A set of any endmembers defines a "polytope" or classification figure (triangle for a three component system, tetrahedron for a four component system, a five-tope" in four dimensions for five component system, et cetera).

Given the dimensionality of the polytope from the Q-mode analysis, the polytope is derived by an iterative process. These procedures are basically exercises in Euclidian geometry. The initial polytope is defined as either the vertices of the K most mutually extreme samples or as k points within the data cloud roughly parallel to the shape of the data cloud. Points lying outside the initial polytope are reported as having negative mixing proportions for one or more endmembers. If this occurs, the polytope iteratively expands and rotates until convergence occurs or the maximum number of iterations is reached. A solution is not guaranteed - and sometimes solutions may diverge.

Inspection of the results for intermediate iterations identifies those samples which are difficult to accommodate within a polytope. Often, the reasons for this are readily apparent in that a subset might represent a distinct subpopulation totally unrelated to the rest of the samples or a subpopulation with extreme geochemical values due to small sample size or analytical error. Discrete subsets can also be detected by the fact that they contain endmembers which are un-needed in the other samples. Such evaluation permits breaking the data into subsets for further analysis. Endmembers variability within a subset often reflects degree of fractionation and assimilation. If major, minor, and trace elements are included in the analysis, the composition of endmembers describes the partitioning of trace elements with respect to majors and minors.

Analysis of two lunar sample data sets (mare, highland) illustrate the manner in which PVA allows classification and analysis of such heterogeneous data.

POLYTOPIC VECTOR ANALYSIS OF LUNAR SAMPLES, J.W. SHERVAIS AND R. ERM

Pristine Highland Cumulates from Western Nearside: Our analysis of cumulate plutonic rocks focused on breccia clasts from the Apollo 14 and Apollo 12 sites [7-10]. The sample set consisted of 31 samples containing 21 chemical elements. All but six samples are related to the Mg-suite (mostly troctolites with a few norites and peridotites); the last six were alkali suite anorthosites and norites. The initial Q-mode analysis indicated that a five endmember solution was best, but that Si and Ba were poorly recovered by back-calculation from that solution. This reflects the fact that these elements are poorly determined analytically; in fact, silica was typically derived by difference from INAA analyses. The Q-mode analysis also indicated that a small subset of samples (primarily alkali anorthosites) would be slightly biased by a five-EM solution. The five EMs represent approximate compositions of olivine (dunite), olivine-pyroxene mix, An100 plagioclase with abundant trace elements, An100 plagioclase with few trace elements, and An86 plagioclase with moderate trace elements. Ultramafic samples commonly fell outside the polytope (large negative mixing proportions). Most Mg-suite samples are characterized by roughly 2:1 ratios of An100 plagioclase to An86 plagioclase EMs producing An95 compositions, with variable amounts of the "dunite" EM to make troctolite. The alkali suite samples are dominated by the An86 plagioclase EM, with small contributions from the trace element-rich "pyroxene" EM. Using just the major elements alone, only a three EM solution can be obtained and was petrologically viable but uninteresting.

Lunar Mare Basalts: When all mare basalts are considered as a class (121 samples with 22 chemical elements), Q-mode analysis of variance suggests that a five EM solution is required. Two of these EMs represent basaltic compositions which bracket mare basalt compositions, Two represent fictive extracts (armalcolite, plagioclase, olivine combinations), and one represents a KREEP-rich ferrobasalt. Thus, our preliminary results suggest that the KREEP component in mare basalts is an Fe-rich ferrobasalt with very low MgO that is fractionated with respect to pristine KREEP 15386. Further work is in progress to determine relations among primitive basalt compositions to constrain mantle source variations.

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